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QUARTERLY

R E P O R T

by

THE OHIO STATE UNIVERSITY
RESEARCH FOUNDATION

1314 Kinnear Road
Columbus 12, Ohio

To: DEPARTMENT OF THE NAVY
Office of Naval Research
Contract No. Nonr 495(12)
ARPA Order No. 23-61; Task 1, Item 4

On: STRUCTURAL AND THERMODYNAMIC PROPERTIES OF POLYATOMIC MOLECULES AT ELEVATED TEMPERATURES

For the period: 1 April 1964 - 30 June 1964

Submitted by: David White
Department of Chemistry

Date: 30 September 1964

STRUCTURAL AND THERMODYNAMIC PROPERTIES OF
POLYATOMIC MOLECULES AT ELEVATED TEMPERATURES

The infrared absorption spectra of magnesium fluoride and magnesium chloride isolated in solid argon and krypton matrices have been investigated in the region 240 to 4000 cm^{-1}. The highest frequency bands for the molecule MgF_2 are observed at 843, 833, and 823 cm^{-1} in solid krypton. These can be assigned to ν_3 of $Mg^{24}F_2$, $Mg^{25}F_2$, and $Mg^{26}F_2$. The magnitude of the isotopic shifts suggests a linear or slightly bent molecular configuration. There is some experimental evidence for the bent configuration, namely, a band in the vicinity of 740 cm^{-1} which may be the symmetric stretch. However it is not clear at the time whether this band can be assigned to the molecular species MgF_2. The lowest frequency band observed in the infrared spectrum of matrix-isolated MgF_2 occurs at 242 cm^{-1} in solid krypton. It can be assigned to the bending mode, ν_2. Regardless of whether MgF_2 is linear or slightly bent, the new frequency assignment yields thermal functions in good agreement with experiments.

In matrix-isolated $MgCl_2$ only one band has been observed which can positively be assigned to this molecule. It occurs at 509 cm^{-1} in solid krypton. This band is probably the asymmetric stretch, ν_3. The bending to frequency for the molecule, ν_2, is estimated to fall in the region 150-1d0 cm^{-1} by analogy with MgF_2. Thermal functions calculated from such an assignment, assuming a linear configuration are in good agreement with experiments. The infrared studies will be extended to lower frequencie when the new Pekin-Elmer Model 301 spectrometer is delivered.

The above infrared absorption studies were presented and discussed at the Symposium on Molecular Spectroscopy and Structure held in Columbus in June.

Some preliminary matrix-isolation studies of the isotopic species BH_3NH_3, BD_3ND_3, were initiated during the quarter. Investigation of the infrared absorption spectra of matrix-isolated CaF_2 and $CaCl_2$ were also started this quarter.

Some progress has been made in the interpretation of the fine structure observed in the infrared spectra of matrix-isolated hydrogen halides. A model which takes into consideration nearest neighbor interactions between the trapped species and the surrounding rare gas atoms has been developed which nearly quantitatively accounts for the observations.

Investigator Dana A. White Date 10/12/64

Supervisor Dana A. White Date 10/12/64

For the Ohio State University Research Foundation

Executive Director Robert C. Stephenson Date 10/12/64

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